Toward a reanalysis of MLS Stratospheric Chemical Observations

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1. Motivations

- BASCOE system provides operational analysis of the stratospheric chemical composition since 2009 using MLS scientific retrievals with a latency of 3-5 days (www.copernicus-stratosphere.eu)
- These analyses are used by WMO Global Atmosphere Watch (GAW) to produce the Arctic and Antarctic Ozone Bulletin
- BASCOE analyses are provided as 6-hourly snapshot and are:
  - easier to interpret the global state of the stratosphere than MLS profiles
  - more accurate than free model output
- A reanalysis of MLS between 2004-present will allow GAW to evaluate more easily the evolution of the polar stratosphere since 2004
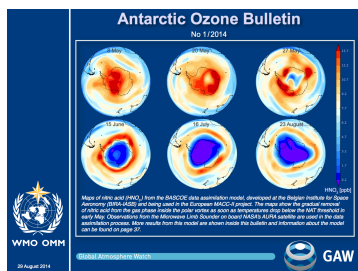

Figure 1: Illustration of use of BASCOE analyses of MLS for the production of the WMO GAW Antarctic Ozone Bulletin. Here is shown the cover page of the 1st bulletin of 2014.

2. Experimental setup

All numerical experiments descibed here have been done with the Belgian Assimilation System for Chemical Observations (BASCOE; Errera et al., ACP, 2008; Skachko et al., GMD, 2016)

- Chemistry Transport Model :
  - 58 stratospheric species advected by the Flux Form Semi Lagrangian (Lin and Rood, MWR, 1996)
  - ~200 chemical reactions (gas-phase, photolysis and heterogeneous)
  - PSC Parameterization of their formation/evaporation, sedimentation and heterogeneous reactions rates on their surface (see box 4)
  - Resolution: 2.5°lat x 3.75°lon x 37 levels between 0.1 hPa - surface
  - Time step: 30'
  - Dynamical fields: ERA-Interim
- Data Assimilation:
  - Method: 4D-Var (Errera et al., ACP, 2008, 2012) or EnKF (Skachko et al., GMD, 2014, 2016). See box 5
  - 4D-Var B matrix assume homogeneous and isotropic spatial Gaussian correlations with length scales L_h=800 km and L_v=1 vertical level
- Observations: Aura MLS v4.2 profiles of O_3, H_2O, HNO_3, N_2O, HCl, ClO and CO according to the Data Quality Document recommendations
- Period of interest: April-November 2008

3. New H_2O setup at the UTLS

- Old setup used ERA-Interim between surface-2 km above tropopause
- BASCOE CTM includes a new setup to account for H_2O condensation which leads to a better agreement with MLS (CTM and DA)
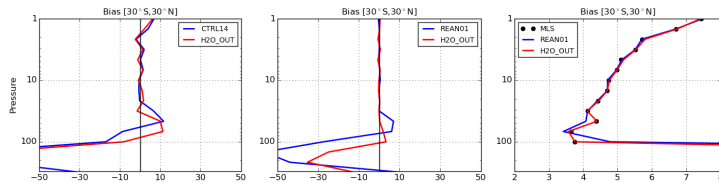

Figure 2a: Mean differences between MLS and CTM with OLD and NEW H_2O setup for one day in 2008 in the Tropics

Figure 2b: Mean differences between MLS and 4D-Var with OLD and NEW H_2O setup for one day in 2008 in the Tropics

Figure 2c: Mean profiles of MLS and 4D-Var with OLD and NEW H_2O setup for one day in 2008 in the Tropics

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4. South Polar Winter Model simulations

Four Chemistry Transport Model (CTM) simulations:

- **CTM 1**: PSC existance as a function of T°. PSC sedimentation assume exponential decay (Errera et al., ACP, 2008):

  If T<186K: $VMR_{HNO3}=VMR_{HNO3}*EXP(-9days* \Delta t)$
                 $VMR_{H2O}=VMR_{H2O}*EXP(-9days* \Delta t)$
                 ICE exist with SAD=10^6 cm^2/cm^3
  Else If T<194K: $VMR_{HNO3}=VMR_{HNO3}*EXP(-100days* \Delta t)$
                 NAT exist with SAD=10^7 cm^2/cm^3

- **CTM 2**: PSC existance as a function of condensation pressure. PSC sedimentation assume exponential decay (Huijnen et al., GMD, 2016, in press):

  If $p_{H2O}>p_{ICE}$: $VMR_{HNO3}=VMR_{HNO3}*EXP(-9days* \Delta t)$
                 $VMR_{H2O}=VMR_{H2O}*EXP(-9days* \Delta t)$
                 ICE exist with SAD=10^6 cm^2/cm^3
  Else If $p_{HNO3}>p_{NAT}$: $VMR_{HNO3}=VMR_{HNO3}*EXP(-20days* \Delta t)$
                 NAT exist with SAD=10^7 cm^2/cm^3

- **CTM 3**: REPROBUS PSC parameterization (Lefèvre et al., JGR, 1994)
- **CTM 4**: As CTM 3 where NAT formation is slowed down

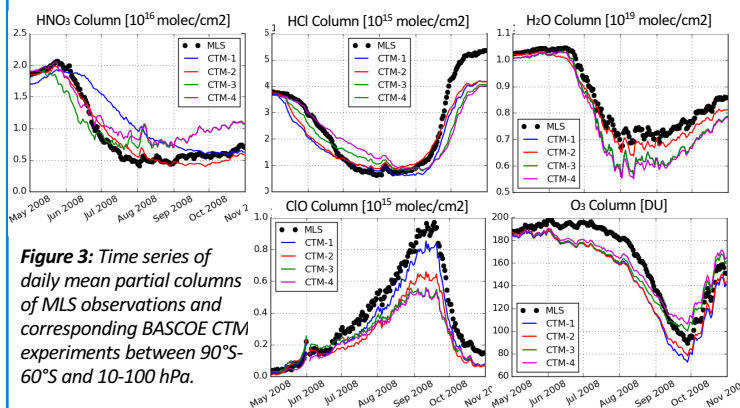*Figure 3: Time series of daily mean partial columns of MLS observations and corresponding BASCOE CTM experiments between 90°S-60°S and 10-100 hPa.*

5. South Polar Winter Data Assimilation Experiments

Four DA simulations:

- **DA 1a**: 4D-Var with PSC setup as in **CTM 1**
- **DA 1b**: EnKF with PSC setup as in **CTM 1**
- **DA 2**: 4D-Var with PSC setup as in **CTM 2**
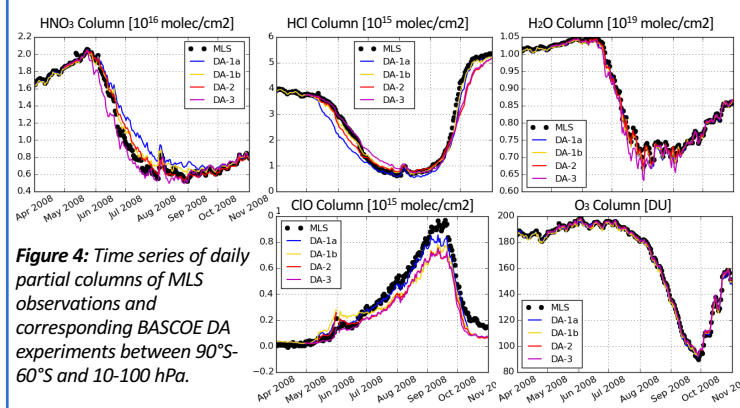- **DA 3**: 4D-Var with PSC setup as in **CTM 4**

Figure 4: Time series of daily partial columns of MLS observations and corresponding BASCOE DA experiments between 90°S-60°S and 10-100 hPa.

6. Conclusions

- None of PSC parameterizations used in CTM or DA agree completely with MLS
- Complex PSC parameterization (e.g. Reprobus) are not necessarily better than simple one
- EnKF seems to perform better than 4D-Var
- Work in progress